

Phase separation in a two species Bose mixture

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We obtain the ground state quantum phase diagram for a two species Bose mixture in a one-dimensional optical lattice using the finite size density matrix renormalization group(FSDMRG) method. We discuss our results for different combinations of inter and intra species interaction strengths with commensurate and incommensurate fillings of the bosons. The phases we have obtained are superfluid, Mott insulator and a novel phase separation, where the two different species reside in spatially separate regions. The spatially separated phase is further classified into phase separated superfluid(PS-SF) and Mott insulator(PS-MI). The phase separation appears for all the fillings we have considered; whenever the inter-species interaction is slightly larger than the intra-species interactions.

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I. INTRODUCTION

Studies of quantum phase transitions are currently of great interest as they provide important insights into a wide variety of many-body systems [1, 2]. The pioneering observation of the superfluid (SF) to Mott insulator (MI) transition in an optical lattice using cold bosonic atoms [3], which had been predicted by Jaksch et. al. [4], highlights the exquisite control of the inter atomic interactions that is possible in such systems. In that experiment, performed using ⁸⁷Rb atoms, the tunneling of the atoms to neighboring sites and also the strength of the on-site interactions were controlled by tuning and/or detuning the laser intensity in order to achieve the transition from the SF phase (random distribution of atoms) to the MI phase where there are a fixed number of atoms per site [3]. Recent developments involving the manipulation of ultracold atoms have led to the realization of genuine one dimensional systems such as the Tonks-Girardeau gas [5]. Several interesting phenomena including the SF-MI transition have been observed in one-dimensional optical lattices [6].

In the past few years, on the theoretical side, many investigations have been carried out using a single species of bosonic atoms in optical lattices [7, 8]. Recently cold bosonic mixtures [9], fermions [10] and Bose-Fermi mixtures [11, 12] in optical lattices have attracted much attention. Mixtures of different species are very interesting since additional phases could appear due to the inter-species interactions [13, 14].

In the present work, we consider a system with two species of bosonic atoms or equivalently, bosonic atoms with two relevant internal states. The two species shall be called *a* and *b* type respectively. The low-energy Hamil-

tonian is then given by the Bose-Hubbard model for the two boson species:

$$H = -t^a \sum_{\langle i,j \rangle} (a_i^\dagger a_j + h.c) - t^b \sum_{\langle i,j \rangle} (b_i^\dagger b_j + h.c) + \frac{U^a}{2} \sum_i n_i^a (n_i^a - 1) + \frac{U^b}{2} \sum_i n_i^b (n_i^b - 1) + U^{ab} \sum_i n_i^a n_i^b. \quad (1)$$

Here a_i (b_i) is bosonic annihilation operator for bosonic atoms of *a* (*b*) type localized on site *i*. $n_i^a = a_i^\dagger a_i$ and $n_i^b = b_i^\dagger b_i$ are the number operators. t^a (t^b) and U^a (U^b) are the hopping amplitudes between adjacent sites $\langle ij \rangle$ and the on-site intra-species repulsive energies, respectively for *a* (*b*) type of atom. The inter-species interaction is given by U^{ab} . The hopping amplitudes (t^a , t^b) and interaction parameters (U^a , U^b , U^{ab}) are related to depth of optical potential, recoil energy and the scattering lengths. The ratio $U^{ab}/U^{a,b}$ can be controlled to a wide range of values [15] experimentally. In this work we consider inter-exchange symmetry $a \leftrightarrow b$, implying $t^a = t^b = t$ and $U^a = U^b = U$ and study the effect of inter-species interaction on the ground state of model(1) in one-dimension. We set our energy scale by $t = 1$.

The model (1) has been studied earlier using the mean field [15], Monte-Carlo [13] and the Bosonization methods [14] and this has resulted in the prediction of the basic structure of its ground state phase diagram. The Bosonization study predicts phase separation (PS) for large values of the inter-species interaction U^{ab} by considering one species of bosons to be hard core and the other to be in the intermediate to hard core regime [14]. Phase separation has also been found using a variational method based on the multi orbital best mean field ansatz [16]. However, a clear picture of the transitions pertaining to the SF, MI and PS phases has not emerged so far. In order to achieve this, we consider the influence of the inter-species interaction U^{ab} on these phases, by carrying out a systematic study of its effect on the ground

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state of model (1) in one-dimension using the finite size density matrix renormalization method [8, 17]. The following part of the paper is organized as follows. Section II contains the details of our finite size density matrix renormalization method. Section III contains our results. We end with concluding remarks in Section IV.

II. FSDMRG CALCULATION

The Finite-Size Density-Matrix Renormalization Group (FSDMRG) method has proven to be very useful in studies of one-dimensional quantum systems[8, 17]. The details of this method are given in a recent review by Schollwöck [18]. The open boundary condition is preferred over periodic boundary condition for this method because the loss of accuracy which increases with the size of the system is much less in the former than the latter. In the conventional FSDMRG method, the lattice is first built to the desired length (L) using the infinite system density-matrix renormalization method (DMRG). The finite size sweeping is done only for this desired lattice size L . We use a slightly modified form of the FSDMRG, where we sweep at *every step* of the procedure and not just for the case which corresponds to the largest value of L . This enables one to obtain accurate correlation functions. Furthermore, since the superfluid phase in models such as Eq. (1), in $d = 1$ and at $T = 0$, is critical and has a correlation length that diverges with the system size L , finite-size effects must be eliminated by using finite-size scaling as we show later. For this purpose, the energies and the correlation functions, obtained from a DMRG calculation, should converge satisfactorily for each system size L . It is important, therefore, that we use the FSDMRG method as opposed to the infinite-system DMRG method especially in the vicinities of continuous phase transitions.

In the FSDMRG method the bases used for left- and right-block Hamiltonians are truncated by neglecting the eigenstates of the density matrix corresponding to small eigenvalues which leads to truncation errors. If we retain M states, the density-matrix weight of the discarded states is $P_M = \sum_{\alpha=1}^M (1 - \omega_\alpha)$, where ω_α are the eigenvalues of density matrix. P_M provides a convenient measure of the truncation errors. We find that these errors depend on the order-parameter and correlation length for a given phase. For a fixed M , we find very small truncation errors in the gapped phase and the truncation errors are largest for the SF phase. In our calculations we choose M such that the truncation error is always less than 5×10^{-5} and we find that $M = 128$ suffices.

The number of possible states per site in the model(1) is infinite since there can be any number of a and b species bosons on a site. In a practical FSDMRG calculation we must truncate the number of states n_{max} allowed per site. The value of n_{max} , of course, will depend on the on-site interaction U . The smaller the value of U the larger must be n_{max} . From our earlier calculation[8] on related

models, we find that $n_{max} = 4$ is sufficient for the value of U considered here. This implies, for model(1), 4 states each per site for a and b species bosons and a total of 16 states per site. This corresponds to a truncation of bases of left (right) block from $16M$ to M in each FSDMRG iteration.

Before proceeding further we give a brief summary of our results. The various parameters that we calculate to study the ground state properties of model (1) are the energy gap G_L , which is the difference between the energies needed to add and remove one atom from a system of atoms,i.e.,

$$G_L = E_L(N_a + 1, N_b) + E_L(N_a - 1, N_b) - 2E_L(N_a, N_b) \quad (2)$$

and the on-site density correlation function

$$\langle n_i^\alpha \rangle = \langle \psi_{0LN_aN_b} | n_i^\alpha | \psi_{0LN_aN_b} \rangle. \quad (3)$$

Here α , is an index representing type a or b bosons, $E_L(N_a, N_b)$ is the ground-state energy for a system of size L with N_a (N_b) number of a (b) type bosons and $|\psi_{0LN_aN_b}\rangle$ is the corresponding ground-state wavefunction, which are obtained by the FSDMRG method. In $d = 1$, the appearance of the MI phase is signaled by the opening up of the gap $G_{L \rightarrow \infty}$. However, G_L is finite for finite systems and we must extrapolate to the $L \rightarrow \infty$ limit, which is best done by using finite-size scaling [8]. In the critical region, i.e., SF region, the gap

$$G_L \approx L^{-1} f(L/\xi), \quad (4)$$

where the scaling function $f(x) \sim x$, $x \rightarrow 0$ and ξ is the correlation length. $\xi \rightarrow \infty$ in the SF region. Thus plots of LG_L versus U , for different system sizes L , consist of curves that intersect at the critical point at which the correlation length for $L = \infty$ diverges and gap G_∞ vanishes.

Defining the ratio of the inter and intra species interactions $\Delta = U^{ab}/U$, we study the ground state of model (1) for $\Delta < 1$, $\Delta = 1$ and $\Delta > 1$. The ground state exhibits some similarities as well as differences in each of the cases. When the kinetic energy is the dominant term in the model, the ground state is in 2SF (both a and b species are in the SF phase) state for all Δ . This similarity is, however, lost when the interactions dominate. For $\Delta \leq 1$, i.e., $U^{ab} \leq U$, the large U phase is Mott insulator with non-zero energy gap in the ground state. This state has a uniform local density of bosons for each species, i.e., $\langle n_i^a \rangle = \langle n_i^b \rangle$ for all i . The 2SF to MI transition is possible only when the total density $\rho = \rho_a + \rho_b$ is an integer. For $U^{ab} \sim U$, the 2SF-MI transition for model (1) is similar to the SF-MI transition for single species bosons with the same density of bosons. For $\Delta > 1$ and for small values of U , the ground state is a 2SF state. However, when U increases, the ground state first goes into superfluid phase with a and b bosons spatially separated into different regions of the lattice. This is the case when $\rho_a = \rho_b = 1/2$. This phase may

be called the phase separated superfluid(PS-SF). There is no gap in the ground state energy spectrum and the phase separation order parameter defined as

$$O_{PS} = \frac{1}{L} \sum_i \langle \psi_{0LN_a N_b} | (|n_i^a - n_i^b|) | \psi_{0LN_a N_b} \rangle. \quad (5)$$

is non-zero. A further increase in U results in opening up of the gap in the energy spectrum. This Mott insulator has a non-zero phase separation order parameter and it may be called the phase separated Mott-Insulator(PS-MI). The total local density $\langle n_i \rangle (= \langle (n_i^a + n_i^b) \rangle) = \rho$ remain uniform across the lattice. When the densities are different, for example $\rho_a = 1$, $\rho_b = 1/2$, no PS-MI is found and the ground state has only 2SF and PS-SF phases. When $\rho_a = 1$, $\rho_b = 1$ we find, for $\Delta = 1.05$, no PS-SF phase and the transition is directly from 2SF to PS-MI. We now present the details of our results.

III. RESULTS AND DISCUSSIONS

In the absence of the inter-species interaction U^{ab} , model (1) is an independent mixture of the individual species of bosons. So the nature of the ground state of model (1) depends only on the density of the individual species of bosons: ρ_a , ρ_b and $U^a = U^b = U$, the on-site interactions. For example, if $\rho_a \neq n$, $\rho_b \neq n$, where n is an integer, the ground state is always in the superfluid phase irrespective of the strength of the on-site interaction U . The Mott insulator is possible only when either $\rho_a = n$ or $\rho_b = n$. Based on the values of ρ_a , ρ_b and U , the ground state is categorized as 2SF (both a and b type bosons in SF phase), SF+MI (a boson in SF and b in MI phase or vice-versa) and MI+MI (both a and b bosons in MI phase). For $\rho_a \neq n$, $\rho_b \neq n$ or for any values of ρ_a , ρ_b , but $U < U_c$, where U_c is the critical on-site interaction for SF to MI transition, the ground state is always in the 2SF phase. SF+MI phase is possible for $\rho_a \neq n$, $\rho_b = n$ (or vice-versa) and $U > U_c$. If both $\rho_a = \rho_b = n$ and $U > U_c$, we have MI+MI phase. In order to investigate the influence of U^{ab} on these ground states, we consider three cases: $\Delta < 1$, $\Delta = 1$ and $\Delta > 1$, where $\Delta = U^{ab}/U$. In each of these three cases, we consider three different ranges of densities: (i) $\rho_a = \rho_b = 1/2$, (ii) $\rho_a = 1, \rho_b = 1/2$, (iii) $\rho_a = \rho_b = 1$. The choice of these three cases are made to understand the effect of the inter-species interaction on 2SF, SF+MI and MI+MI phases. We now discuss each case below.

(i) $\rho_a = \rho_b = 1/2$:

As discussed in the previous paragraph, for this case, there is no MI phase if $U^{ab} = 0$ and the model (1) will have only the 2SF phase. However, with the introduction of inter-species interaction, the 2SF phase is destroyed. For example, Figure (1) shows a plot of scaling of gap LG_L versus U for $\Delta = 1$. Curves for different values of L coalesce for $U \leq U_c \simeq 3.4$ indicating a gapped MI phase for $U > U_c$. The emergence of this phase is due to the

intra-species as well as interspecies interaction strengths. The fact that $U_c \simeq 3.4$, indicates that the model (1) when $\Delta = 1$ behaves like a single species of bosons at unit density [8]. These results are along the expected lines because, when $U^{ab} = U$, every boson in the system interacts with rest of bosons, irrespective of whether they are of type a or b , with the same strength and therefore the species index become irrelevant. However, the situation changes when the inter-species interaction $U^{ab} \neq U$.

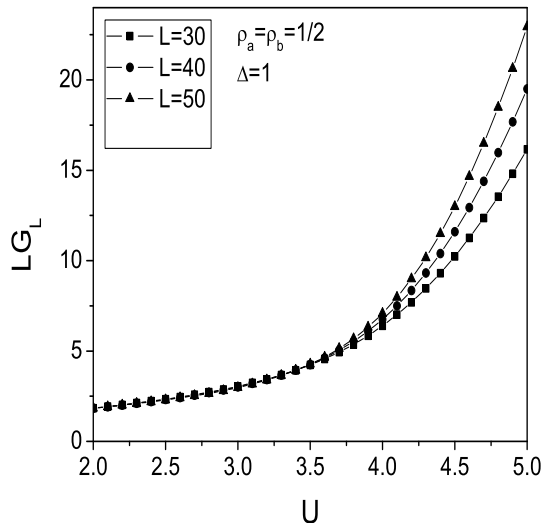


FIG. 1: Scaling of gap LG_L is plotted as a function of U for different system sizes for $\rho_a = \rho_b = 1/2$, $\Delta = 1$. The coalescence of different curve for $U \leq 3.4$ shows a Kosterlitz-Thouless-type 2SF-MI transition. This transition is similar to the SF-MI transition for single species Bose-Hubbard model for $\rho = 1$ [8].

For $\Delta < 1$, i.e., $U^{ab} < U$, the system still undergoes 2SF-MI transition when the on-site repulsion increases, but with a higher U_c . For example figure (2) shows a plot of scaling of gap LG_L versus U for $\Delta = 0.5$. The critical $U_c(\Delta = 0.5) \sim 5.4$ is substantially greater than $U_c(\Delta = 1) \sim 3.4$. The ground state of the model(1) for $\rho_a = \rho_b = 1/2$, $\Delta < 1$ consists only of 2SF and MI phases. The transition from 2SF to MI is of Kosterlitz-Thouless-type.

When $\Delta > 1$, the scenario is drastically different from the one seen above. The on-site densities $\langle n_i^a \rangle$ and $\langle n_i^b \rangle$ are plotted in Fig. (3) for $\Delta = 1.05$. It is clear from this figure that there is a spatial separation between the two different species of bosons for $U = 4$ and no spatial separation for $U = 1$. This highlights a *phase separation* (PS) transition as a function of U . The question then arises whether this spatially separated phase is a superfluid or a Mott Insulator. In order to sort this out, we plot both the scaling of the gap LG_L and the order parameter O_{PS} for phase separation in Fig. (4). It is evident from these figures that the transition to the MI

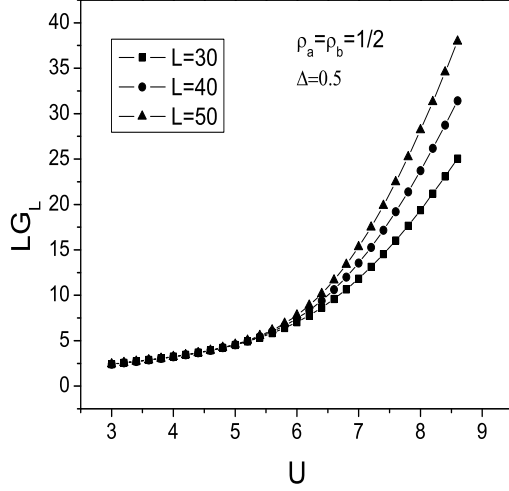


FIG. 2: Scaling of gap LG_L is plotted as a function of U for different system sizes for $\rho_a = \rho_b = 1/2$, $\Delta = 0.5$. The coalescence of different curve for $U \simeq 5.4$ shows a Kosterlitz-Thouless-type 2SF-MI transition.

phase happens at around $U_c \simeq 3.4$ and to the spatially separated phase around $U_c \simeq 1.3$. The gap remains zero for $1.3 < U < 3.4$. Thus for the case $\rho_a = \rho_b = 1/2$ and $\Delta = 1.05$, there are three phases: the superfluid phase (2SF) for $U < 1.3$, superfluid, but phase separated (PS-SF) for $1.3 < U < 3.4$ and finally Mott Insulator, but again phase separated (PS-MI) for $U > 3.4$. It should be noted that the total density of bosons $\rho = \rho_a + \rho_b$ remain constant through out the lattice, though bosons are space separated. The critical values of 2SF to PS-SF and PS-SF to PS-MI transition depends of the on the value of Δ . The detailed phase diagram in the $\Delta - U$ plane and the nature of the different phase transitions will be reported elsewhere.

(ii) $\rho_a = 1, \rho_b = 1/2$:

In this case, when $U^{ab} = 0$ species a bosons undergo a superfluid to Mott insulator transition at $U_c \simeq 3.4$ by virtue of having density $\rho_a = 1$, while the b bosons, which has density $\rho_b = 1/2$, remains in the superfluid phase. However, when $U^{ab} \leq U$, no transition from SF to MI was found for either of the two species of bosons. The Mott insulator phase of a bosons is completely lost. In the Fig. (5(a)), we plot the length dependence of gap G_L for different U , which clearly indicates that the gap vanishes at $L \rightarrow \infty$ for all values of U considered. This emphasizes the fact that as far as the transition to the Mott insulator is concerned, when $U^{ab} \leq U$, the total density must be an integer irrespective of the densities of the individual species of bosons; and it is this condition that really matters. This condition remains same for $U^{ab} > U$. Thus when the inter-species interaction is non zero as in the present case and the total density $\rho \neq n$,

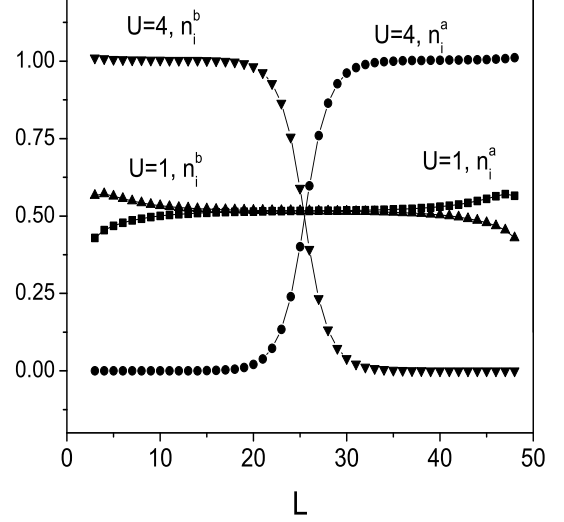


FIG. 3: Plots of $\langle n_i^a \rangle$ and $\langle n_i^b \rangle$ versus i for $U = 1$ and $U = 4$. These plots are for $\rho_a = \rho_b = 1/2$, $\Delta = 1.05$ and for system size $L = 50$. The deviation in $\langle n_i^a \rangle$ and $\langle n_i^b \rangle$ near the boundaries for $U = 1$ is due to the open boundary condition used in our FSDMRG.

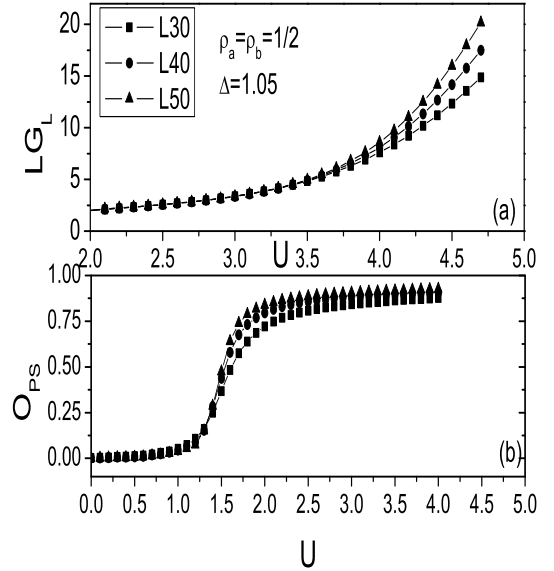


FIG. 4: Plots of scaling of gap LG_L (a) and order parameter for phase separation O_{PS} (b) versus U demonstrate various phases for the case $\rho_a = \rho_b = 1/2$ and $\Delta = 1.05$.

no Mott insulator phase is observed.

The phase separation, however, happens when $U^{ab} > U$. The local density distribution of different species of bosons are given in Fig. (5(b)) for $U = 1, 4$ and $\Delta = 1.05$. For $U = 1$, we find no phase separation, however, for $U = 4$, the a and b species bosons are phase separated. They rearrange in such a manner that the total density $\rho = \rho_a + \rho_b$ remains a constant. For example, when $\rho_a = 1$ and $\rho_b = 1/2$, one-third of the region is occupied by the species b and two-third by the species a . The total density ρ being $3/2$, the distributions of the a and b types of bosons follow the ratio of their densities.

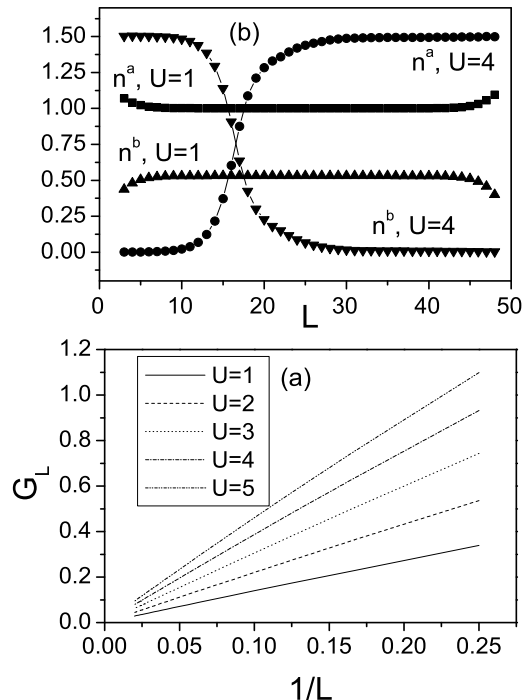


FIG. 5: (a) Plots of gap G_L versus $1/L$ for different values of U . The gap goes to zero linearly when $L \rightarrow \infty$ for all the values of U considered. Here $\rho_a = 1$, $\rho_b = 1/2$ and $\Delta = 0.95$. (b) Local density distribution $\langle n_i^a \rangle$ and $\langle n_i^b \rangle$ for $\rho_a = 1$, $\rho_b = 1/2$ and $\Delta = 1.05$ for two different $U = 1, 4$.

(iii) $\rho_a = 1, \rho_b = 1$:

Finally we consider double commensurate case where both the species of bosons undergo SF to MI phase transition in the absence of U^{ab} . It may be noted that for $\rho_a = \rho_b = 1$, $U_c \sim 3.4$ for $U^{ab} = 0$. In Fig. (6), we plot the scaling of the gap LG_L for $\Delta = 1.0$. From this figure and from similar ones for $\Delta \leq 1$ i.e., $U^{ab} \leq U$, we find that the transition from 2SF to MI occurs at a much higher value of $U = U_c \sim 5.7$. No SF-MI transition observed at $U \sim 3.4$. Due to the collective intra and inter species interactions in model (1), the species index become irrelevant for the phase transition. For $U^{ab} \sim U$, the phase transition from 2SF to MI is similar to the SF-MI transition in single species bosons with density $\rho = 2$.

This is consistent with the similar observations made for the case of $\rho_a = \rho_b = 1/2$.

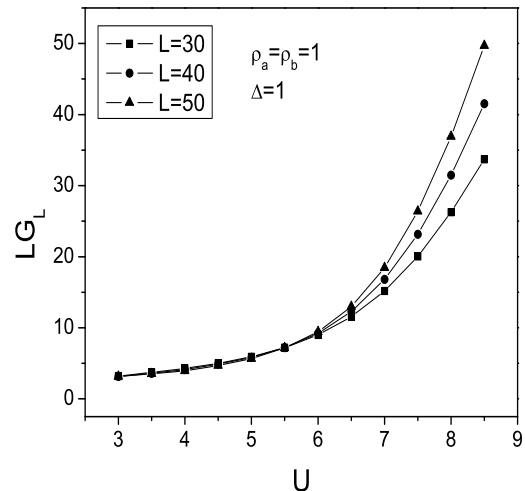


FIG. 6: Scaling of gap LG_L is plotted as a function of U for different system sizes for $\rho_a = \rho_b = 1$ and $\Delta = 1.0$. The coalescence of different curve for $U \simeq 5.7$ shows a Kosterlitz-Thouless-type 2SF-MI transition.

The phase separation transition, however, occurs for $\Delta \gtrsim 1$ as given in the Fig. (7). In this case the transitions to phase separation and to the Mott insulator occur around same $U_c \sim 5.7$. In other words we did not find a PS-SF phase sandwiched between 2SF and PS-MI for this case.

IV. CONCLUSION

We have studied the ground state of a two species Bose mixture in one dimension using the finite-size density-matrix renormalization group method. We have considered three sets of densities $\{\rho_a, \rho_b\} = \{1/2, 1/2\}, \{1, 1/2\}, \{1, 1\}$. Analyzing the scaling of gap in the energy spectrum and the order parameter for phase separation we have obtained several phases: 2SF, MI, PS-SF and PS-MI. For $U^{ab} \leq U$, the Mott Insulator phase is possible only when the total density $\rho = \rho_a + \rho_b = n$, is an integer. The superfluid to Mott Insulator transition in model (1) is then similar to the single species Bose-Hubbard model with the same total density ρ . The critical on-site interaction for the 2SF-MI transition, however, depends on the values of Δ . The lower the value of Δ , the larger the value of U_c . For $\rho \neq n$, Mott insulator phase is not found. Phase separation occurs for $U^{ab} > U$ irrespective of the value of density. For $\rho = n$ and for all the values of Δ that we have considered, we found phase separated Mott insulator phase. In the case of $\rho_a = \rho_b = 1/2$, we observe a phase separated superfluid

PS-SF sandwiched between 2SF and PS-MI. However, for $\rho_a = \rho_b = 1$, no PS-SF was found and the transition is directly from 2SF to PS-MI. For $\rho_a = 1, \rho_b = 1/2$ we found a transition from 2SF to PS-SF for $\Delta > 1$ and only 2SF phase for $\Delta \leq 1$. It would indeed be worthwhile to devise experiments to test our findings.

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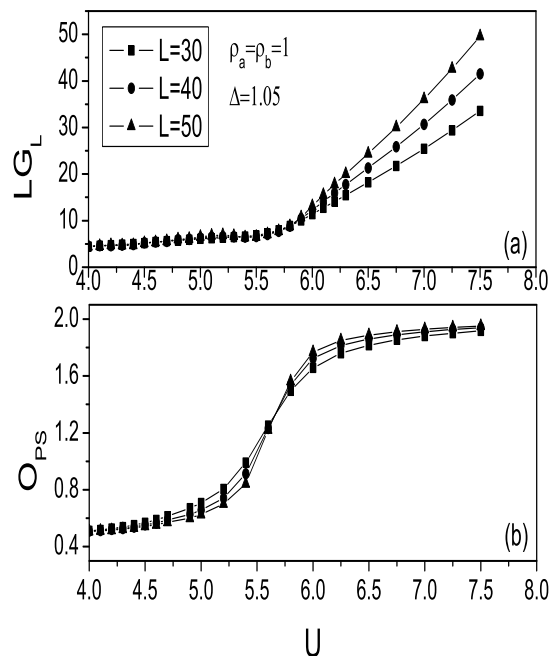


FIG. 7: Plots of LG_L (a) and O_{PS} (b) versus U demonstrate various phases in the case of $\rho_a = \rho_b = 1$, $\Delta = 1.05$.

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